2014 NERSC Workload Analysis

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Understanding the NERSC workload is key to procuring productive, high performing systems for science.

- Conducted workload analysis to understand application requirements and guide future system procurements.
- Important for understanding efforts needed to transition workload to future architectures.
- Analyzed the workload by:
  - Science area
  - Application code
  - Algorithm
  - Job size
  - Thread usage
  - Memory usage
  - Library usage
  - I/O usage
Workload analysis aims to understand how users exercise the available computational resources.

NERSC engages in other activities to complement the workload analysis.

- Requirement reviews ascertain the future needs of users.
- Benchmarking and performance analysis reveals performance characteristics and sensitivities of individual applications.
- Workflow analysis describes the operational and data dependencies of a single project. (The workload is a cross-section of many simultaneous workflows.)

Requirements for future procurements are obtained by combining all these sources of information. A retrospective workload analysis reflects current (not future) hardware and software resource utilization.
Data collected in this presentation came from a variety of sources.

• System accounting logs
• NIM database
• ALPS command line capture log
• Automatic Library Tracking Database (ALTD)
• Resource Utilization Report (RUR)
• Lustre Monitoring Tool (LMT)
## Current (and imminent !) NERSC systems.

<table>
<thead>
<tr>
<th></th>
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</tr>
</thead>
<tbody>
<tr>
<td>Interconnect</td>
<td>6384 nodes Cray Gemini (3D Torus)</td>
<td>5576 nodes Cray Aries (Dragonfly)</td>
<td>9300 KNL nodes plus 1624 Haswell nodes Cray Aries (Dragonfly)</td>
</tr>
<tr>
<td>Processor</td>
<td>Two 12-core AMD Magny Cours (2.1 GHz)</td>
<td>Two 12-core Intel Ivy-Bridge (2.4 GHz)</td>
<td>One 64+ core Intel Knight’s Landing (GHz TBD)</td>
</tr>
<tr>
<td>Memory</td>
<td>32 GB/node; 54 GB/s</td>
<td>64 GB/node; 102 GB/s</td>
<td>96 GB DDR4/node; 90 GB/s 16 GB HBM; &gt;400 GB/s</td>
</tr>
<tr>
<td>Scratch Filesystem</td>
<td>2.0 PB; 70 GB/s</td>
<td>7.5 PB; 168 GB/s</td>
<td>28.5 PB; &gt;700 GB/s Burst Buffer: 1.5 PB; 1.5 TB/s</td>
</tr>
<tr>
<td>Sustained System Performance*</td>
<td>144 Tflop/s</td>
<td>293 Tflop/s</td>
<td>&gt;10 x Hopper</td>
</tr>
</tbody>
</table>

Workload Diversity
Workload diversity questions:

• Which science domains and algorithms are represented in the applications at NERSC?
• What codes, libraries and languages are most important to NERSC users?
NERSC serves a broad range of science disciplines for the DOE Office of Science

- Over 5950 users
- Nearly 850 projects

Top 5 Science Categories by allocation (2014)

<table>
<thead>
<tr>
<th>Category</th>
<th>Percentage</th>
</tr>
</thead>
<tbody>
<tr>
<td>Materials Science</td>
<td>20%</td>
</tr>
<tr>
<td>Fusion Energy</td>
<td>18%</td>
</tr>
<tr>
<td>Chemistry</td>
<td>12%</td>
</tr>
<tr>
<td>Climate Research</td>
<td>11%</td>
</tr>
<tr>
<td>Lattice QCD</td>
<td>11%</td>
</tr>
</tbody>
</table>
Over 650 applications run on NERSC resources

Top Application codes on Hopper and Edison by hours used.
Jan – Dec 2014

• 13 codes make up 50% of workload
• 25 codes make up 66% of workload
• 50 codes make up 80% of workload
• Remaining codes (over 600) make up 20% of workload.
Many codes implement similar algorithms.

- Regrouped top codes by similar algorithms.

- A small number of benchmarks can represent a large fraction of the workload.

- Includes Genepool and PDSF systems.
  - Carver was similar in size to PSDF, but had a diverse workload.
Languages Used at NERSC

Fraction of codes using various languages - 2015 (not weighted by hours used)

- Fortran
- C++
- C
- Python*
- Assembler
- UPC

* - Job/Workflow management & production code

- Based on user surveys.
- Fortran would be even more important if codes were weighted by hours used.
  - Fortran is the primary language for 23 of the 36 top codes.
- Total exceeds 100% because some codes use multiple languages.
NERSC’s broad workload relies on optimized libraries to maximize performance.

Top 15 libraries used on Edison (2014)

- libsci
- scalapack
- hdf5
- mkl
- fftw
- fftw3
- netcdf
- hdf5-parallel
- dmapp
- metis
- superlu
- parallelmetis
- mumps
- superlu_dist
- petsc
NERSC enables a prodigious volume of scientific research.

• Over 1800 publications during 2014
Concurrency
Parallelism and Concurrency

- What are common job sizes at NERSC?
- How are users expressing parallelism in their codes?
- Users will likely need threads to take full advantage of many-core architectures like Cori. How much is OpenMP used now?
High concurrency jobs are a significant fraction of the NERSC workload.

- 37% of Edison hours use more than 16 K cores.
- 4% of Edison hours use more than 2/3 of its cores.

### Edison Job Size Breakdown (2014)

<table>
<thead>
<tr>
<th>Cores Used</th>
<th>Core Hours</th>
</tr>
</thead>
<tbody>
<tr>
<td>&gt;64K</td>
<td>7%</td>
</tr>
<tr>
<td>16K-64K</td>
<td>31%</td>
</tr>
<tr>
<td>4K-16K</td>
<td>17%</td>
</tr>
<tr>
<td>1K-4K</td>
<td>18%</td>
</tr>
<tr>
<td>1-1K</td>
<td>25%</td>
</tr>
<tr>
<td>1</td>
<td>2%</td>
</tr>
</tbody>
</table>
High concurrency jobs are used in all science domains.

- Some fraction of every domain’s workload runs with more than 16K cores.
High concurrency jobs are used in all science domains.

- Some fraction of every domain’s workload runs with more than 16K cores.
- In almost all domains, more than half the workload uses more than 1K cores.
High concurrency jobs are used in all science domains.

- Some fraction of every domain’s workload runs with more than 16K cores.
- In almost all domains, more than half the workload uses more than 1K cores.
- Does not include the Genepool or PDSF clusters.
  - Combined, these are 7% of the workload.
Nearly all projects rely on MPI for distributed memory parallel programming.

Fraction of codes using various parallel programming models.

- Based on user survey of codes used. Not weighted by core hours.
- Total exceeds 100% because some codes use multiple languages.
- 40% of projects report using OpenMP.
NERSC users are embracing threads.

<table>
<thead>
<tr>
<th></th>
<th>Hopper</th>
<th>Edison</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fraction of hours</td>
<td>14%</td>
<td>21%</td>
</tr>
<tr>
<td>using OpenMP</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- Currently nearly 20% of hours are consumed using multiple OpenMP threads.
- Thread concurrency has increased over generations of systems.
- On both systems, the dominant thread concurrency matches the NUMA domain.
  - Hopper: 6 cores per NUMA domain
  - Edison: 12 cores per NUMA domain
High concurrency jobs use more threads.

- Thread utilization increases with node count.
  - More than half of the core hours using 2/3 of Edison are threaded. (not shown)

- Thread concurrency increases with node count.
  - Jobs with 12 threads per process is dominate at higher concurrency.

- OpenMP use increases at large scales where MPI scaling inefficiencies outweigh (on-node) OpenMP inefficiencies.
Summary

• Users need to run single-node jobs, full-system jobs, and everything in between.
  – 37% of the Edison workload use more than 16k cores
  – 75% uses more than 1024 cores.

• MPI is (still) the predominant form of parallelism in user codes.

• About 20% of the workload uses threads.
  – OpenMP adoption has increased over system generations.
  – Thread utilization increases with node count.
  – Thread concurrency seems to match NUMA domain size.
Memory utilization
Memory utilization

• How much memory is being used per node? Per MPI rank?
• Edison has twice as much memory per node as Hopper. How often is it used?
• What fraction of the NERSC workload will fit into Cori’s HBM without modification?
• Limited memory (and HBM) capacity was a potential motivator for thread adoption. Is this reflected by current OpenMP use?
Users are taking advantage of Edison’s increased memory per node.

- Hopper has 32 GB nodes, Edison has 64 GB nodes
- 8% of Edison workload uses more than 80% of available memory per node.
- 16% of the Edison workload would not run on Hopper’s 32 GB nodes.*
- 71% of Edison workload will fit into Cori’s fast memory (16 GB).

*Assuming MPI+X concurrency does not change.
A modest fraction (10%) of the Edison workload uses more than 4 GB per MPI rank.

- Most Edison users are not constrained by memory capacity.
  - 15% of Edison hours use more than 2.6 GB / rank.
  - Of this 15%, four threaded codes make up 60%.
  - Much of the remaining 40% is sequential code

- Many users run a handful of large memory jobs.
OpenMP adoption does not seem to be driven by limited memory capacity.

- Only a small fraction (<5%) of multi-threaded jobs use more than 80% of available memory.
- Most (>95%) multi-threaded jobs have sufficient memory to accommodate an additional MPI rank per node.
- No simple relationship between thread concurrency and memory use.
Memory capacity summary

• About 1/6\textsuperscript{th} Edison’s workload could not fit into Hopper’s 32 GB nodes.

• About half of the Edison workload will have no problems running exclusively in Cori’s HBM (assuming no changes).

• OpenMP adoption does not seem to be driven by limited memory capacity.
Storage and I/O
Storage and I/O questions

- What are the biggest I/O issues effecting users?
- What are the read and write volumes of filesystem activity?
- How much of the I/O load is due to checkpointing?
- How quickly are NERSC filesystems filling?
- What is the distribution of file sizes?
More reliable metadata performance would improve application performance.

- Cron job times “ls” and file creation every five minutes to test I/O metadata performance on Edison’s scratch1 filesystem.
- Benchmarks normally complete in 2 or 3 seconds.
- More than one in five tests are significantly slower.
- Both benchmarks have long tails stretching to 300s.
I/O bandwidth variation degrades quality of service

- Cron job measures performance of IOR benchmark each week.
- I/O benchmarks routinely measure large fractions of peak bandwidth.
- “Typical” measurements are 25-40% slower.
  - 30-50% variation
  - A few runs are much slower.
Users seldom achieve large fractions of peak I/O bandwidth.

- Lustre Monitoring Tool (LMT) counts total data read/written within 5 second intervals.
- Even poorly performing benchmark runs exceed the I/O rates observed in production.*
  - No file system exceeds 10% of peak more than 10% of the time.
  - 99% of /scratch3 samples use less than 20 GB/s (27% of peak).
  *Actual I/O rates may exceed the inferred rates. (Large sampling window)

- Significant fractions of peak are routinely measured.
  - See benchmark results on previous slide.
  - 63 of 812,000 LMT samples exceed 80% of peak on Edison’s /scratch3.
Maximum daily write volume \( \approx 2 \times \) memory capacity.

- LMT measurements of data read/written each day, summed over scratch filesystems.
- Read/write balance shifts from Hopper to Edison.
  - Read volume is similar between systems.
  - Edison has 3x write volume.

### Average daily scratch I/O volume (TB)

<table>
<thead>
<tr>
<th></th>
<th>Read</th>
<th>Write</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hopper</td>
<td>139.8</td>
<td>105.2</td>
</tr>
<tr>
<td>Edison</td>
<td>139.4</td>
<td>303.0</td>
</tr>
</tbody>
</table>
Much of the NERSC workload seems to use checkpoint-restart functionality.

- A large fraction (70%) of core hours is consumed by jobs that reach the wallclock limit.
  - Steps in plot correspond to queue limits.
- Users want longer queues (and shorter wait times)
- 95% of jobs run for less than one hour.
Edison has three scratch filesystems.

Users are randomly assigned to either `/scratch1` or `/scratch2`
- Performance isolation
- Improved metadata performance

Users with demanding I/O requirements may opt-in to `/scratch3`.
- 1.5x bandwidth
- 1.5x capacity
- Default striping increased for better bandwidth.
- Additional performance isolation

<table>
<thead>
<tr>
<th>Filesystem</th>
<th>/scratch1</th>
<th>/scratch2</th>
<th>/scratch3</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>Capacity (TB)</td>
<td>2100</td>
<td>2100</td>
<td>3200</td>
<td>7400</td>
</tr>
<tr>
<td>Bandwidth (GB/s)</td>
<td>48</td>
<td>48</td>
<td>72</td>
<td>168</td>
</tr>
</tbody>
</table>
Edison scratch filesystem utilization increases 10 TB/day.

- Linear growth of /scratch1 and /scratch2
  - 12 week purge policy
  - 1 TB quota per user

- /scratch3 growth is less predictable.
  - Piecewise linear?
  - 8 week purge policy
  - No quota
  - Fills more than 2x faster than /scratch1 or /scratch2

96% of data written to scratch is for temporary use.
  - Average write volume is ~300 TB/day.
  - Aggregate growth of data stored is ~10 TB per day.

<table>
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<th>/scratch2</th>
<th>/scratch3</th>
<th>Total</th>
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<td>72</td>
<td>168</td>
</tr>
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</table>
Project filesystem utilization increases 5 TB/day.

- "Project" is a large, permanent, medium performance filesystem.
- Project directories are intended to facilitate sharing data among users and across NERSC systems.
- Linear growth
  - No purge policy
  - 1 TB quota per project
Total NERSC file-system utilization increases 15 TB/day.

- **Linear growth**
  - Summed over filesystems
  - Various quota and purge policies

<table>
<thead>
<tr>
<th>Capacity (TB)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Global homes</td>
</tr>
<tr>
<td>Global project</td>
</tr>
<tr>
<td>Global projectb</td>
</tr>
<tr>
<td>Global scratch</td>
</tr>
<tr>
<td>Hopper scratch</td>
</tr>
<tr>
<td>Hopper scratch2</td>
</tr>
<tr>
<td>Edison scratch1</td>
</tr>
<tr>
<td>Edison scratch2</td>
</tr>
<tr>
<td>Edison scratch3</td>
</tr>
</tbody>
</table>
Files on Edison’s scratch filesystems are generally small.

- Average size: 9.4 MB
- Most (70%) files smaller than the 1 MB Lustre stripe size.
- Vast majority (>97%) of files smaller than 32 MB.
- Most (>90%) data is in files larger than 1MB.

<table>
<thead>
<tr>
<th>Total Count</th>
<th>Total Volume</th>
<th>Min</th>
<th>Max</th>
</tr>
</thead>
<tbody>
<tr>
<td>91 M</td>
<td>821 TB</td>
<td>0 B</td>
<td>5 TB</td>
</tr>
</tbody>
</table>
File sizes on /project are similar to Edison’s /scratch2.

- Average size: 8.1 MB
- Most (80%) files smaller than the 1 MB.
- Most (>90%) data is in files larger than 1MB.
Storage and I/O summary

- I/O metadata and bandwidth performance are highly variable.
- Users seldom see the I/O rates they expect.
- Edison’s maximum daily write volume is about twice its memory capacity. Hopper reads more data than Edison, sometimes 3x memory capacity per day.
- About 70% of the workload seems to use checkpoint/restart to cope with queue walltime limits.
- Filesystem utilization increases roughly linearly (15 TB/day).
- Most files (70%) are smaller than 1 MB. Most data (>90%) is in files larger than 1 MB.
Conclusions

• NERSC supports many users, domains and algorithms, and has a broad scientific impact.

• Most codes are still written Fortran, C++, or C, with MPI parallelism. OpenMP thread usage is 20%.
  – For large jobs, any OpenMP inefficiencies are outweighed by MPI scalability issues.
  – Among threaded codes, the dominant thread concurrency matches the NUMA domain size.

• Few Edison users are constrained by memory capacity.
  – Half of the Edison workload will run in Cori’s 16 GB HBM without modification.

• Users seldom achieve large fractions of I/O bandwidth on scratch filesystems.
  – Checkpoint – restart is common.
  – Maximum daily write volume is about 2x memory capacity.
  – Filesystem utilization grows steadily at 15 TB/day.
Over 650 applications run on NERSC resources.

- 10 codes make up 45% of workload
- 25 codes make up 66% of workload
- 50 codes make up 80% of workload
- Remaining codes (over 600) make up 20% of workload.

Top Application codes on Hopper and Edison by hours used. Jan – Dec 2014

Alternative chart format; Labels are more readable & assignable, but pie size does not match format of other slides.
NERSC’s broad workload relies on optimized libraries to maximize performance.

Library usage on Edison by number of unique users (1/13/2014 - 1/12/2015)
VASP and ESPRESSO Usage At NERSC Over Time

Percentage of Cycles at NERSC

Year

- 48 -
Adoption of threads varies across disciplines.

Fraction of Edison core hours used

Threads
- 2
- 4
- 6
- 12
- 24
- 48
Science domains have different concurrency needs.
Users choose Edison for running jobs with large aggregate memory footprints.

- When given more powerful nodes and networks, users take advantage of increased memory (but not always at full-system scale).
- Memory capacity does not constrain Edison’s largest jobs.
  - Largest job uses only 2/3 memory; 10th largest uses 1/3 memory.
  - Edison’s largest jobs could not fit on Hopper.

95% of Edison core hours are used by jobs that use less than 32 TB.
More reliable metadata performance would improve application performance variation.

- Cron job times “ls” and file creation every five minutes to test I/O metadata performance on Edison’s scratch1 filesystem.
- Benchmarks normally complete in 2 or 3 seconds.
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Much of the NERSC workload relies on checkpoint-restart functionality.

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  - Steps in plot correspond to queue limits.
  - This is only 0.5% of jobs.

- Users want longer queues (and shorter wait times)

  95% of jobs run for less than one hour.